



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:55 AM UTC

PDB ID : 1MWS / pdb_00001mws
Title : Structure of nitrocefin acyl-Penicillin binding protein 2a from methicillin resistant *Staphylococcus aureus* strain 27r at 2.00 Å resolution.
Authors : Lim, D.C.; Strynadka, N.C.J.
Deposited on : 2002-10-01
Resolution : 2.00 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

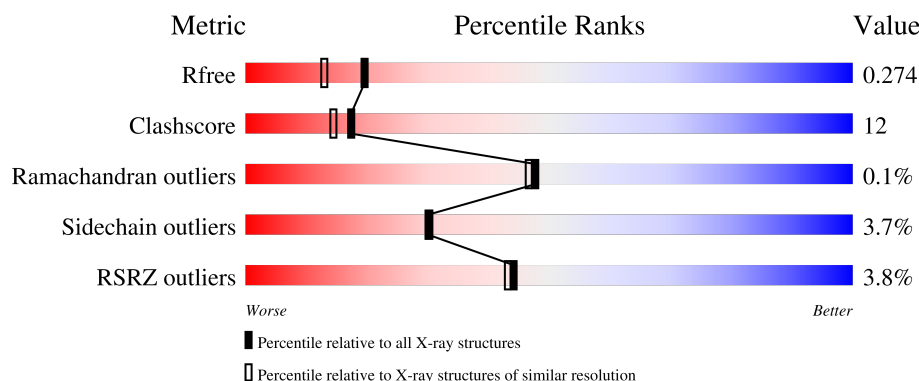
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	646	3% 72% 24% ..
1	B	646	4% 74% 21% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called penicillin-binding protein 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5130	3235	861	1017	17			
1	B	629	Total	C	N	O	S	0	0	0
			5056	3192	850	999	15			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cd	0	0
			5	5		
2	B	3	Total	Cd	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		

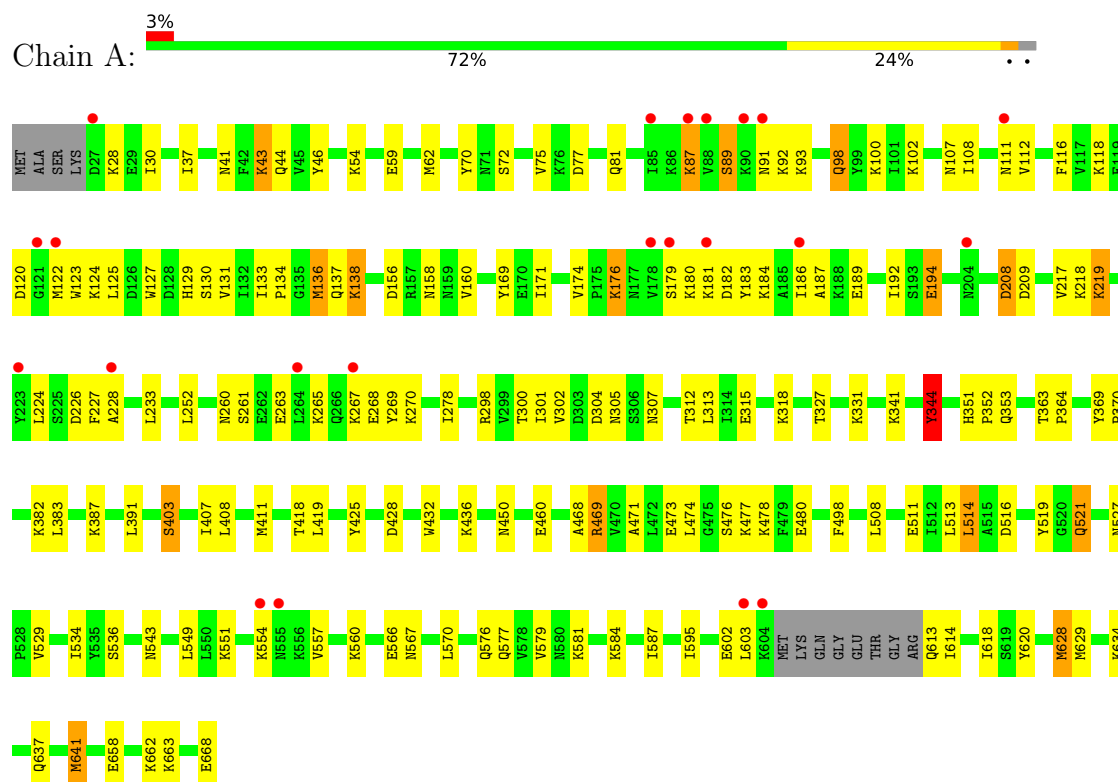
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		
4	B	189	Total	O	0	0
			189	189		

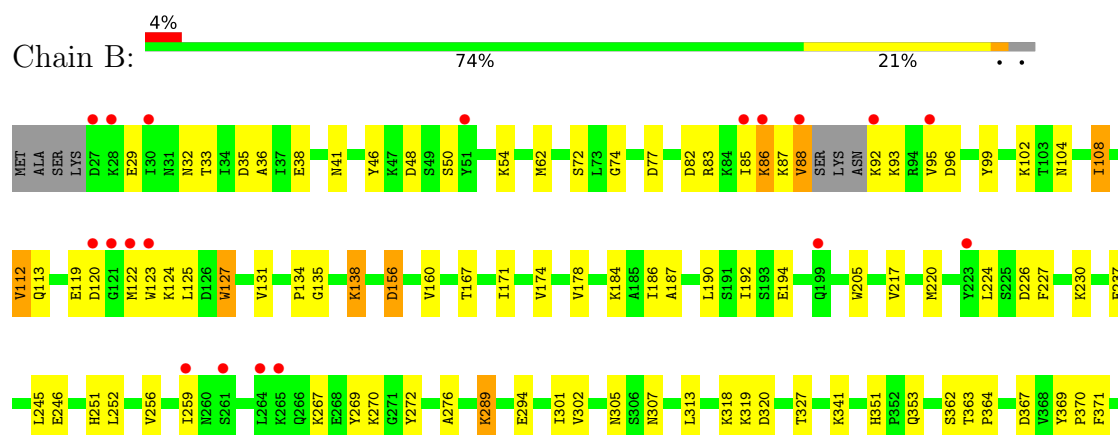
3 Residue-property plots [i](#)

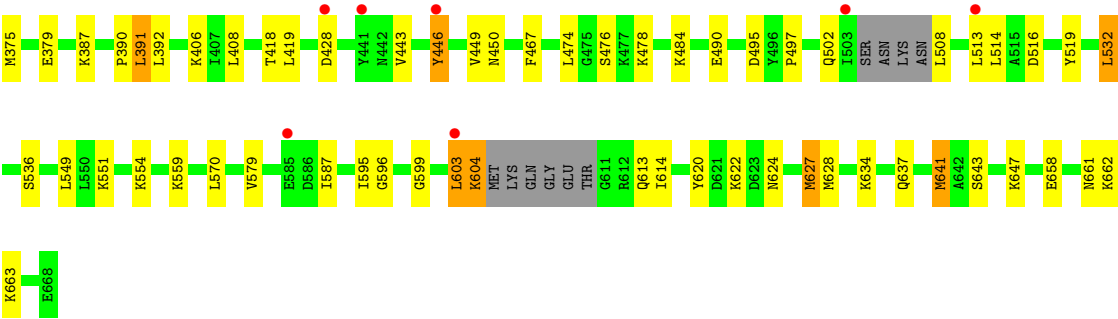
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: penicillin-binding protein 2a



• Molecule 1: penicillin-binding protein 2a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.58Å 100.75Å 187.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.00 24.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (24.96-2.00) 96.6 (24.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.274 0.236 , 0.274	Depositor DCC
R_{free} test set	5059 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10592	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NC1, CL, CD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	1/5173 (0.0%)	0.99	16/6955 (0.2%)
1	B	0.55	0/5132	1.00	19/6897 (0.3%)
All	All	0.56	1/10305 (0.0%)	1.00	35/13852 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	MET	SD-CE	-8.11	1.59	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	VAL	N-CA-C	-10.38	96.14	107.77
1	A	174	VAL	N-CA-C	-9.65	97.27	107.60
1	A	641	MET	CB-CA-C	-8.08	107.25	116.54
1	A	468	ALA	N-CA-C	-7.43	103.26	111.36
1	A	351	HIS	CA-C-N	7.25	128.90	119.84
1	A	351	HIS	C-N-CA	7.25	128.90	119.84
1	A	219	LYS	N-CA-C	6.98	120.89	109.72
1	B	127	TRP	N-CA-C	6.96	120.05	110.24
1	B	246	GLU	CB-CA-C	-6.91	108.59	116.54
1	B	341	LYS	N-CA-C	6.87	120.54	111.75
1	B	178	VAL	N-CA-C	6.77	117.59	108.11
1	A	341	LYS	N-CA-C	6.28	118.93	111.33
1	B	641	MET	CB-CA-C	-6.03	109.64	116.63
1	A	218	LYS	N-CA-C	5.94	117.43	111.07
1	B	418	THR	N-CA-C	-5.82	105.95	113.16
1	A	301	ILE	N-CA-C	-5.78	99.42	107.80
1	A	418	THR	N-CA-C	-5.61	106.10	113.17
1	B	351	HIS	CA-C-N	5.51	125.60	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	HIS	C-N-CA	5.51	125.60	119.32
1	A	628	MET	N-CA-C	-5.50	100.22	109.07
1	B	246	GLU	N-CA-C	5.50	116.67	108.31
1	B	596	GLY	N-CA-C	5.48	118.58	110.42
1	A	344	TYR	N-CA-C	-5.42	100.95	109.25
1	B	131	VAL	N-CA-C	-5.41	104.98	112.50
1	B	599	GLY	N-CA-C	5.41	118.35	112.29
1	B	160	VAL	N-CA-C	-5.35	102.68	109.58
1	B	301	ILE	N-CA-C	-5.33	100.07	107.80
1	B	443	VAL	N-CA-C	-5.29	100.97	108.58
1	A	169	TYR	N-CA-C	5.24	117.44	108.90
1	A	160	VAL	N-CA-C	-5.16	102.86	109.30
1	A	194	GLU	N-CA-C	-5.11	105.79	111.36
1	B	108	ILE	N-CA-C	-5.11	101.05	108.36
1	A	511	GLU	N-CA-C	5.07	116.81	111.28
1	B	497	PRO	N-CA-C	5.04	119.10	110.74
1	B	495	ASP	N-CA-C	-5.02	106.75	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5130	0	5105	144	0
1	B	5056	0	5049	119	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	205	0	0	7	0
4	B	189	0	0	3	0
All	All	10592	0	10154	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:H	1:B:138:LYS:HD2	1.13	1.07
1:A:138:LYS:H	1:A:138:LYS:HD2	1.38	0.87
1:B:226:ASP:O	1:B:230:LYS:HG2	1.75	0.85
1:B:387:LYS:HA	1:B:387:LYS:HE2	1.57	0.84
1:A:138:LYS:H	1:A:138:LYS:CD	1.89	0.84
1:B:184:LYS:HG2	1:B:194:GLU:OE1	1.79	0.82
1:A:87:LYS:H	1:A:87:LYS:HD3	1.42	0.82
1:B:604:LYS:HA	1:B:604:LYS:HE3	1.59	0.82
1:B:267:LYS:HA	1:B:270:LYS:HG3	1.59	0.81
1:A:133:ILE:HB	1:A:136:MET:HE2	1.64	0.80
1:B:138:LYS:H	1:B:138:LYS:CD	1.93	0.80
1:A:112:VAL:HG11	1:A:134:PRO:HB3	1.62	0.79
1:A:658:GLU:HG3	1:A:662:LYS:HD3	1.65	0.78
1:A:176:LYS:HG3	1:A:208:ASP:O	1.84	0.78
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.15	0.77
1:A:603:LEU:HD22	1:A:613:GLN:N	2.00	0.77
1:A:179:SER:OG	1:A:181:LYS:HB3	1.86	0.75
1:A:576:GLN:HG2	4:A:1154:HOH:O	1.87	0.75
1:A:480:GLU:HG3	1:A:508:LEU:HD12	1.69	0.74
1:A:176:LYS:HD2	1:B:113:GLN:NE2	2.02	0.73
1:A:602:GLU:HG2	1:A:613:GLN:HE22	1.54	0.72
1:B:86:LYS:HG2	1:B:87:LYS:H	1.54	0.72
1:B:87:LYS:O	1:B:88:VAL:HG13	1.91	0.70
1:B:88:VAL:HG23	1:B:92:LYS:O	1.92	0.70
1:B:579:VAL:HG13	1:B:587:ILE:HG23	1.74	0.69
1:A:138:LYS:HE3	4:A:1151:HOH:O	1.91	0.69
1:B:138:LYS:HD2	1:B:138:LYS:N	1.98	0.69
1:A:187:ALA:HB1	1:A:192:ILE:O	1.93	0.69
1:B:220:MET:HE2	1:B:220:MET:HA	1.76	0.67
1:A:637:GLN:O	1:A:641:MET:HE1	1.96	0.66
1:B:29:GLU:OE1	1:B:123:TRP:HD1	1.77	0.66
1:A:176:LYS:HB2	1:A:176:LYS:NZ	2.11	0.65
1:A:89:SER:HB3	1:A:92:LYS:HB3	1.80	0.64
1:A:516:ASP:HA	1:A:519:TYR:CE2	2.33	0.64
1:B:99:TYR:HB2	1:B:112:VAL:HG22	1.79	0.64
1:A:138:LYS:HD2	1:A:138:LYS:N	2.11	0.64
1:A:268:GLU:HG3	1:A:269:TYR:CD1	2.33	0.63
1:B:627:MET:O	1:B:627:MET:HG3	1.97	0.63
1:B:370:PRO:HB2	1:B:375:MET:HE2	1.80	0.63
1:A:403:NC1:O31	1:A:403:NC1:H4	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:GLU:CG	1:A:662:LYS:HD3	2.29	0.63
1:A:554:LYS:HD3	1:A:554:LYS:H	1.63	0.62
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.82	0.61
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.65	0.61
1:A:91:ASN:ND2	1:A:118:LYS:HB3	2.14	0.61
1:B:449:VAL:HG23	1:B:449:VAL:O	2.01	0.61
1:A:184:LYS:HB3	1:A:194:GLU:CD	2.25	0.61
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.30	0.61
1:B:614:ILE:HD11	1:B:634:LYS:HG3	1.84	0.60
1:B:318:LYS:HE3	1:B:320:ASP:OD2	2.02	0.60
1:A:179:SER:C	1:A:181:LYS:H	2.08	0.60
1:B:251:HIS:HE1	1:B:390:PRO:O	1.84	0.60
1:B:536:SER:HA	1:B:628:MET:HE1	1.82	0.60
1:B:536:SER:HA	1:B:628:MET:CE	2.32	0.59
1:A:46:TYR:O	1:A:54:LYS:HD3	2.02	0.58
1:B:86:LYS:C	1:B:87:LYS:HG2	2.28	0.58
1:A:112:VAL:CG1	1:A:134:PRO:CB	2.81	0.58
1:A:180:LYS:HA	1:A:183:TYR:CE1	2.38	0.58
1:A:432:TRP:CH2	1:A:469:ARG:HD3	2.39	0.57
1:B:87:LYS:C	1:B:88:VAL:HG22	2.29	0.57
1:A:383:LEU:HB3	1:A:391:LEU:HD11	1.85	0.57
1:B:108:ILE:HD13	1:B:313:LEU:HD13	1.87	0.57
1:B:38:GLU:OE1	1:B:83:ARG:NH2	2.38	0.57
1:A:557:VAL:HG11	1:A:560:LYS:HG2	1.85	0.57
1:A:602:GLU:HG2	1:A:613:GLN:NE2	2.19	0.57
1:B:85:ILE:HG12	1:B:95:VAL:HG22	1.87	0.57
1:A:87:LYS:H	1:A:87:LYS:CD	2.15	0.57
1:B:614:ILE:HD13	1:B:634:LYS:HA	1.86	0.57
1:A:37:ILE:HD13	1:A:131:VAL:HG13	1.86	0.56
1:A:300:THR:HG22	1:A:312:THR:HA	1.87	0.56
1:B:96:ASP:OD1	1:B:113:GLN:HG2	2.06	0.56
1:A:352:PRO:HA	1:A:536:SER:HB2	1.87	0.56
1:A:81:GLN:NE2	1:A:100:LYS:NZ	2.55	0.55
1:A:137:GLN:HB3	1:A:138:LYS:HD2	1.88	0.55
1:B:294:GLU:OE2	1:B:319:LYS:NZ	2.40	0.55
1:A:81:GLN:NE2	1:A:100:LYS:HZ1	2.05	0.54
1:A:176:LYS:HD2	1:B:113:GLN:HE21	1.72	0.54
1:B:220:MET:CE	1:B:224:LEU:HD23	2.38	0.54
1:A:70:TYR:HB3	1:A:75:VAL:CG2	2.37	0.54
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.42	0.54
1:B:267:LYS:H	1:B:267:LYS:HD3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD13	1:A:313:LEU:HD13	1.90	0.53
1:B:256:VAL:HG22	4:B:1161:HOH:O	2.07	0.53
1:A:77:ASP:HB2	1:A:102:LYS:HE2	1.89	0.53
1:A:261:SER:O	1:A:265:LYS:HG2	2.08	0.53
1:B:93:LYS:HG3	1:B:123:TRP:CZ2	2.44	0.53
1:A:344:TYR:CD1	1:A:344:TYR:C	2.87	0.53
1:B:86:LYS:HB2	1:B:86:LYS:NZ	2.23	0.53
1:A:577:GLN:NE2	1:A:581:LYS:HE2	2.24	0.53
1:B:595:ILE:HD11	1:B:620:TYR:CZ	2.44	0.53
1:A:460:GLU:OE1	1:A:581:LYS:HE3	2.09	0.53
1:A:382:LYS:HD3	1:A:382:LYS:C	2.34	0.52
1:A:432:TRP:CZ2	1:A:469:ARG:HD3	2.44	0.52
1:B:614:ILE:CD1	1:B:634:LYS:HA	2.38	0.52
1:B:171:ILE:HD11	1:B:220:MET:HE1	1.90	0.52
1:B:476:SER:HB3	1:B:508:LEU:O	2.10	0.52
1:A:387:LYS:NZ	1:A:387:LYS:HB3	2.25	0.52
1:B:217:VAL:HG21	1:B:220:MET:HE3	1.92	0.52
1:B:624:ASN:CG	1:B:663:LYS:HE3	2.35	0.52
1:B:48:ASP:O	1:B:124:LYS:HD2	2.10	0.51
1:B:86:LYS:HB2	1:B:86:LYS:HZ2	1.75	0.51
1:A:138:LYS:H	1:A:138:LYS:CE	2.24	0.51
1:B:50:SER:O	1:B:54:LYS:HG3	2.11	0.51
1:B:406:LYS:HG2	1:B:467:PHE:CD1	2.46	0.51
1:B:267:LYS:HA	1:B:270:LYS:CG	2.36	0.50
1:A:407:ILE:O	1:A:411:MET:HG3	2.11	0.50
1:A:603:LEU:HD23	1:A:603:LEU:N	2.26	0.50
1:B:502:GLN:NE2	1:B:502:GLN:HA	2.26	0.50
1:A:122:MET:HE2	1:A:124:LYS:NZ	2.26	0.50
1:A:91:ASN:HD22	1:A:118:LYS:HB3	1.74	0.50
1:A:363:THR:HA	1:A:364:PRO:C	2.36	0.50
1:B:87:LYS:HD2	1:B:93:LYS:HG2	1.93	0.50
1:B:48:ASP:C	1:B:124:LYS:HD2	2.37	0.49
1:B:119:GLU:O	1:B:120:ASP:C	2.55	0.49
1:A:551:LYS:HB2	4:A:1121:HOH:O	2.12	0.49
1:B:637:GLN:HA	1:B:641:MET:SD	2.52	0.49
1:A:305:ASN:O	1:B:72:SER:HB2	2.12	0.49
1:B:251:HIS:CD2	1:B:362:SER:HB3	2.47	0.49
1:A:179:SER:C	1:A:181:LYS:N	2.66	0.49
1:A:603:LEU:HD23	1:A:603:LEU:H	1.78	0.49
1:B:643:SER:O	1:B:647:LYS:HG3	2.12	0.48
1:B:41:ASN:HB3	4:B:1030:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:HB2	1:A:102:LYS:CE	2.44	0.48
1:A:584:LYS:NZ	4:A:1180:HOH:O	2.46	0.48
1:A:111:ASN:OD1	1:A:111:ASN:N	2.47	0.48
1:A:527:ASN:OD1	1:A:529:VAL:HB	2.13	0.47
1:A:93:LYS:HE2	1:A:123:TRP:CE2	2.49	0.47
1:B:363:THR:HA	1:B:364:PRO:C	2.39	0.47
1:A:30:ILE:HD11	1:A:93:LYS:HE3	1.96	0.47
1:B:604:LYS:HA	1:B:604:LYS:CE	2.39	0.47
1:B:46:TYR:O	1:B:54:LYS:HD3	2.15	0.47
1:B:190:LEU:O	1:B:192:ILE:HG23	2.15	0.47
1:A:298:ARG:HD3	1:A:315:GLU:OE1	2.15	0.47
1:A:543:ASN:OD1	1:A:560:LYS:HA	2.15	0.47
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.49	0.47
1:A:269:TYR:CE2	1:A:278:ILE:HD12	2.50	0.47
1:A:217:VAL:HG21	1:A:224:LEU:HD13	1.96	0.46
1:B:474:LEU:O	1:B:478:LYS:HB2	2.15	0.46
1:B:613:GLN:CG	1:B:641:MET:HE1	2.45	0.46
1:A:30:ILE:HG23	1:A:116:PHE:CE1	2.50	0.46
1:B:513:LEU:HD13	1:B:513:LEU:O	2.15	0.46
1:A:318:LYS:NZ	4:A:1172:HOH:O	2.45	0.46
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.50	0.46
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.97	0.46
1:A:471:ALA:HB1	1:A:514:LEU:CD2	2.46	0.46
1:B:187:ALA:HB1	1:B:192:ILE:O	2.16	0.46
1:B:302:VAL:CG1	1:B:307:ASN:HA	2.46	0.46
1:A:176:LYS:HD2	1:B:113:GLN:HE22	1.79	0.46
1:A:182:ASP:O	1:A:186:ILE:HG13	2.15	0.46
1:A:658:GLU:CD	1:A:662:LYS:HD3	2.41	0.46
1:A:498:PHE:CE2	1:A:529:VAL:HG21	2.51	0.45
1:A:77:ASP:CB	1:A:102:LYS:HE2	2.46	0.45
1:B:167:THR:HG23	1:B:237:GLU:HG3	1.97	0.45
1:A:41:ASN:ND2	1:A:44:GLN:HB2	2.30	0.45
1:A:62:MET:HE3	1:A:127:TRP:CG	2.51	0.45
1:A:72:SER:HB2	1:B:305:ASN:O	2.16	0.45
1:B:86:LYS:NZ	1:B:86:LYS:CB	2.78	0.45
1:B:428:ASP:HA	1:B:450:ASN:OD1	2.17	0.45
1:B:613:GLN:HG3	1:B:641:MET:HE1	1.99	0.45
1:B:86:LYS:HG2	1:B:87:LYS:N	2.27	0.45
1:B:603:LEU:HD11	1:B:634:LYS:HE2	1.97	0.45
1:A:158:ASN:OD1	1:B:551:LYS:NZ	2.40	0.45
1:A:70:TYR:HB3	1:A:75:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:HB3	1:B:305:ASN:HB3	1.99	0.45
1:B:35:ASP:OD1	1:B:83:ARG:NH1	2.38	0.45
1:A:179:SER:HB3	1:A:182:ASP:OD1	2.17	0.45
1:A:613:GLN:N	4:A:1088:HOH:O	2.50	0.45
1:A:662:LYS:C	1:A:663:LYS:HD2	2.42	0.45
1:B:82:ASP:OD1	1:B:82:ASP:O	2.34	0.45
1:A:521:GLN:CA	1:A:521:GLN:HE21	2.29	0.44
1:A:577:GLN:HE21	1:A:581:LYS:HE2	1.82	0.44
1:A:436:LYS:H	1:A:436:LYS:HG2	1.49	0.44
1:B:513:LEU:HD13	1:B:513:LEU:C	2.42	0.44
1:A:70:TYR:HB3	1:A:75:VAL:HG21	1.98	0.44
1:A:369:TYR:HB2	1:A:370:PRO:HD3	1.99	0.44
1:B:327:THR:OG1	1:B:549:LEU:HA	2.18	0.44
1:B:391:LEU:HB2	4:B:1066:HOH:O	2.17	0.44
1:A:327:THR:OG1	1:A:549:LEU:HA	2.16	0.44
1:B:86:LYS:O	1:B:87:LYS:HG2	2.16	0.44
1:B:138:LYS:CD	1:B:138:LYS:N	2.69	0.44
1:A:603:LEU:H	1:A:603:LEU:CD2	2.31	0.44
1:B:484:LYS:HB2	1:B:484:LYS:HE3	1.62	0.44
1:A:156:ASP:C	1:A:156:ASP:OD2	2.60	0.44
1:B:93:LYS:HG3	1:B:123:TRP:CH2	2.52	0.44
1:A:260:ASN:O	1:A:263:GLU:HB2	2.18	0.44
1:A:614:ILE:CD1	1:A:634:LYS:HG3	2.48	0.43
1:A:176:LYS:HB2	1:A:176:LYS:HZ1	1.81	0.43
1:A:180:LYS:HA	1:A:183:TYR:CD1	2.54	0.43
1:A:476:SER:O	1:A:477:LYS:C	2.58	0.43
1:A:566:GLU:HG3	1:A:567:ASN:N	2.33	0.43
1:A:425:TYR:OH	1:A:473:GLU:HG3	2.18	0.43
1:B:353:GLN:OE1	1:B:353:GLN:N	2.45	0.43
1:A:129:HIS:HB3	1:A:136:MET:HG2	1.99	0.43
1:A:428:ASP:HA	1:A:450:ASN:OD1	2.18	0.43
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.99	0.43
1:B:251:HIS:CE1	1:B:390:PRO:O	2.70	0.43
1:B:220:MET:HE1	1:B:224:LEU:HD23	2.00	0.43
1:B:269:TYR:HA	1:B:272:TYR:CD1	2.54	0.43
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.53	0.43
1:A:112:VAL:HG12	1:A:134:PRO:CB	2.48	0.43
1:B:371:PHE:CE1	1:B:375:MET:HE1	2.54	0.43
1:B:33:THR:O	1:B:36:ALA:HB3	2.19	0.43
1:B:205:TRP:CD1	1:B:205:TRP:H	2.37	0.43
1:B:369:TYR:HB2	1:B:370:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:GLU:OE1	1:B:559:LYS:NZ	2.47	0.42
1:A:270:LYS:HE2	1:A:270:LYS:HB3	1.90	0.42
1:B:112:VAL:HG13	1:B:134:PRO:CB	2.50	0.42
1:A:353:GLN:H	1:A:353:GLN:CD	2.27	0.42
1:A:474:LEU:O	1:A:478:LYS:HB2	2.19	0.42
1:A:620:TYR:HB3	1:A:628:MET:HG2	2.01	0.42
1:A:668:GLU:OE2	1:B:554:LYS:HD3	2.19	0.42
1:B:375:MET:HG2	1:B:379:GLU:HB2	2.01	0.42
1:B:614:ILE:CD1	1:B:634:LYS:HG3	2.50	0.42
1:A:102:LYS:HA	1:A:107:ASN:OD1	2.20	0.42
1:B:184:LYS:HG2	1:B:194:GLU:CD	2.43	0.42
1:A:614:ILE:HD13	1:A:634:LYS:HA	2.01	0.42
1:A:521:GLN:HA	1:A:521:GLN:NE2	2.35	0.42
1:A:549:LEU:C	1:A:549:LEU:HD12	2.45	0.42
1:B:62:MET:HE3	1:B:127:TRP:CG	2.55	0.42
1:A:100:LYS:HA	1:A:108:ILE:O	2.19	0.42
1:A:304:ASP:O	1:A:305:ASN:HB2	2.20	0.42
1:B:217:VAL:CG2	1:B:220:MET:HE3	2.50	0.42
1:B:289:LYS:HB2	1:B:289:LYS:NZ	2.35	0.42
1:A:28:LYS:HD3	4:A:1183:HOH:O	2.19	0.41
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.02	0.41
1:A:184:LYS:HB3	1:A:194:GLU:OE2	2.19	0.41
1:A:536:SER:HA	1:A:628:MET:CE	2.50	0.41
1:B:259:ILE:HG22	1:B:276:ALA:O	2.21	0.41
1:A:120:ASP:O	1:A:120:ASP:CG	2.63	0.41
1:A:98:GLN:OE1	1:A:98:GLN:HA	2.16	0.41
1:A:352:PRO:HD2	1:A:353:GLN:OE1	2.20	0.41
1:B:613:GLN:CD	1:B:641:MET:HE1	2.45	0.41
1:A:267:LYS:O	1:A:270:LYS:HG3	2.21	0.41
1:A:93:LYS:HE2	1:A:123:TRP:CZ2	2.55	0.41
1:A:209:ASP:OD1	1:B:135:GLY:HA2	2.21	0.41
1:A:219:LYS:H	1:A:219:LYS:HD2	1.86	0.41
1:A:331:LYS:HE3	1:A:668:GLU:OXT	2.20	0.41
1:A:383:LEU:HB3	1:A:391:LEU:CD1	2.49	0.41
1:B:74:GLY:HA3	1:B:104:ASN:ND2	2.36	0.41
1:B:77:ASP:HB3	1:B:102:LYS:HD3	2.02	0.41
1:B:93:LYS:HZ3	1:B:123:TRP:NE1	2.19	0.41
1:A:268:GLU:HG3	1:A:269:TYR:CE1	2.56	0.41
1:A:302:VAL:CG1	1:A:307:ASN:HA	2.50	0.41
1:A:403:NC1:C25	1:A:641:MET:HG3	2.51	0.41
1:A:579:VAL:HG13	1:A:587:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD11	1:A:217:VAL:HG11	2.03	0.40
1:B:406:LYS:NZ	1:B:446:TYR:OH	2.54	0.40
1:B:551:LYS:O	1:B:551:LYS:HD2	2.22	0.40
1:B:658:GLU:HB2	1:B:661:ASN:HB2	2.04	0.40
1:A:43:LYS:HE2	1:A:59:GLU:OE2	2.22	0.40
1:A:618:ILE:HA	1:A:629:MET:O	2.22	0.40
1:B:532:LEU:HD21	1:B:628:MET:HB3	2.03	0.40
1:B:587:ILE:O	1:B:587:ILE:HG12	2.21	0.40
1:B:156:ASP:OD2	1:B:156:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	629/646 (97%)	607 (96%)	22 (4%)	0	100	100
1	B	620/646 (96%)	596 (96%)	23 (4%)	1 (0%)	43	42
All	All	1249/1292 (97%)	1203 (96%)	45 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	MET

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/575 (98%)	548 (97%)	18 (3%)	34	35
1	B	560/575 (97%)	536 (96%)	24 (4%)	26	25
All	All	1126/1150 (98%)	1084 (96%)	42 (4%)	30	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	87	LYS
1	A	89	SER
1	A	98	GLN
1	A	125	LEU
1	A	130	SER
1	A	138	LYS
1	A	176	LYS
1	A	208	ASP
1	A	226	ASP
1	A	252	LEU
1	A	344	TYR
1	A	419	LEU
1	A	469	ARG
1	A	513	LEU
1	A	514	LEU
1	A	521	GLN
1	A	570	LEU
1	B	32	ASN
1	B	86	LYS
1	B	88	VAL
1	B	112	VAL
1	B	125	LEU
1	B	138	LYS
1	B	156	ASP
1	B	245	LEU
1	B	252	LEU
1	B	289	LYS
1	B	367	ASP
1	B	391	LEU
1	B	392	LEU
1	B	408	LEU
1	B	419	LEU
1	B	446	TYR

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Mol	Chain	Res	Type
1	B	514	LEU
1	B	532	LEU
1	B	570	LEU
1	B	603	LEU
1	B	604	LYS
1	B	622	LYS
1	B	627	MET
1	B	662	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	41	ASN
1	A	79	ASN
1	A	81	GLN
1	A	91	ASN
1	A	113	GLN
1	A	115	ASN
1	A	177	ASN
1	A	207	GLN
1	A	305	ASN
1	A	342	ASN
1	A	452	ASN
1	A	457	GLN
1	A	521	GLN
1	A	540	ASN
1	A	555	ASN
1	A	576	GLN
1	A	577	GLN
1	A	593	ASN
1	A	613	GLN
1	A	645	ASN
1	B	32	ASN
1	B	41	ASN
1	B	44	GLN
1	B	79	ASN
1	B	81	GLN
1	B	159	ASN
1	B	177	ASN
1	B	199	GLN
1	B	251	HIS

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Mol	Chain	Res	Type
1	B	342	ASN
1	B	351	HIS
1	B	396	GLN
1	B	415	ASN
1	B	433	GLN
1	B	457	GLN
1	B	502	GLN
1	B	555	ASN
1	B	576	GLN
1	B	645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	NC1	B	403	1	4,5,44	0.83	0	1,5,61	0.65	0
1	NC1	A	403	1	40,43,44	3.34	14 (35%)	39,59,61	1.58	5 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NC1	B	403	1	-	0/2/4/55	-
1	NC1	A	403	1	-	6/30/53/55	0/2/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	NC1	O35-N33	8.63	1.37	1.22
1	A	403	NC1	C4-C5	8.37	1.54	1.37
1	A	403	NC1	O32-N30	8.13	1.36	1.22
1	A	403	NC1	C28-C27	5.59	1.49	1.38
1	A	403	NC1	C11-N10	5.56	1.45	1.34
1	A	403	NC1	C25-N30	-5.50	1.35	1.45
1	A	403	NC1	C29-C24	5.10	1.49	1.41
1	A	403	NC1	C26-C25	4.91	1.48	1.39
1	A	403	NC1	C27-N33	-4.57	1.34	1.45
1	A	403	NC1	C4-C19	4.38	1.55	1.48
1	A	403	NC1	O21-C19	-2.95	1.22	1.30
1	A	403	NC1	C9-N10	2.41	1.50	1.45
1	A	403	NC1	O34-N33	2.33	1.50	1.35
1	A	403	NC1	OG-C7	2.23	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	NC1	C6-S1-C2	5.00	103.52	94.36
1	A	403	NC1	C26-C25-C24	-3.91	119.02	123.09
1	A	403	NC1	O21-C19-C4	-2.81	112.28	116.73
1	A	403	NC1	C24-C23-C22	-2.79	121.44	126.91
1	A	403	NC1	CB-OG-C7	-2.18	111.52	116.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	403	NC1	C-CA-CB-OG
1	A	403	NC1	N-CA-CB-OG
1	A	403	NC1	N10-C11-C13-C14
1	A	403	NC1	O12-C11-C13-C14
1	A	403	NC1	C11-C13-C14-S15
1	A	403	NC1	C11-C13-C14-C18

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	403	NC1	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	633/646 (97%)	0.20	22 (3%) 47 46	19, 34, 56, 75	0
1	B	628/646 (97%)	0.22	26 (4%) 41 40	22, 35, 60, 72	0
All	All	1261/1292 (97%)	0.21	48 (3%) 44 43	19, 35, 58, 75	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	VAL	5.1
1	A	223	TYR	4.5
1	A	121	GLY	4.4
1	B	223	TYR	4.2
1	B	446	TYR	3.8
1	A	603	LEU	3.7
1	A	91	ASN	3.5
1	A	179	SER	3.4
1	A	228	ALA	3.2
1	A	204	ASN	3.1
1	B	28	LYS	3.0
1	A	90	LYS	2.7
1	A	178	VAL	2.7
1	B	121	GLY	2.7
1	B	261	SER	2.6
1	B	85	ILE	2.6
1	B	199	GLN	2.6
1	B	122	MET	2.6
1	A	27	ASP	2.6
1	B	264	LEU	2.6
1	A	181	LYS	2.5
1	B	585	GLU	2.5
1	A	267	LYS	2.5
1	A	604	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	503	ILE	2.5
1	A	122	MET	2.4
1	A	186	ILE	2.4
1	A	111	ASN	2.3
1	B	92	LYS	2.3
1	B	30	ILE	2.3
1	A	88	VAL	2.3
1	B	428	ASP	2.3
1	B	265	LYS	2.3
1	A	85	ILE	2.3
1	B	120	ASP	2.2
1	B	51	TYR	2.2
1	B	27	ASP	2.2
1	A	87	LYS	2.2
1	B	123	TRP	2.2
1	A	554	LYS	2.1
1	B	86	LYS	2.1
1	B	441	TYR	2.1
1	B	603	LEU	2.1
1	A	555	ASN	2.1
1	A	264	LEU	2.1
1	B	513	LEU	2.1
1	B	95	VAL	2.1
1	B	259	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NC1	A	403	41/42	0.89	0.13	25,39,57,61	0
1	NC1	B	403	6/42	0.95	0.07	26,27,29,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	A	1008	1/1	0.94	0.15	100,100,100,100	0
2	CD	B	1006	1/1	0.95	0.09	65,65,65,65	0
3	CL	A	1011	1/1	0.97	0.04	31,31,31,31	0
2	CD	B	1007	1/1	0.98	0.06	52,52,52,52	0
3	CL	B	1009	1/1	0.98	0.04	24,24,24,24	0
3	CL	B	1012	1/1	0.98	0.04	31,31,31,31	0
3	CL	A	1010	1/1	0.99	0.04	27,27,27,27	0
2	CD	A	1004	1/1	0.99	0.06	50,50,50,50	0
2	CD	A	1003	1/1	1.00	0.02	30,30,30,30	0
2	CD	B	1002	1/1	1.00	0.01	26,26,26,26	0
2	CD	A	1001	1/1	1.00	0.02	26,26,26,26	0
2	CD	A	1005	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.